

A Recurrent Neural Network-based Surrogate Model for History-Dependent Multi-scale Simulations

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Computational & Multiscale Mechanics of Materials

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COMPLAS 21

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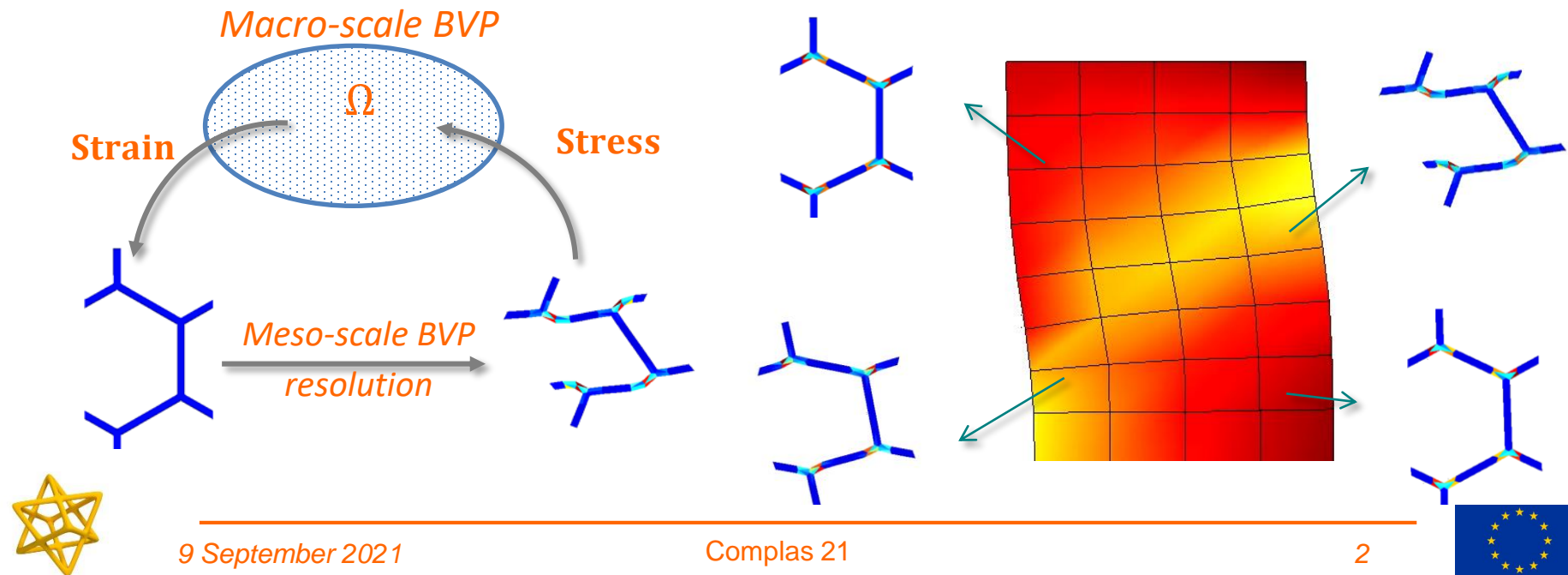
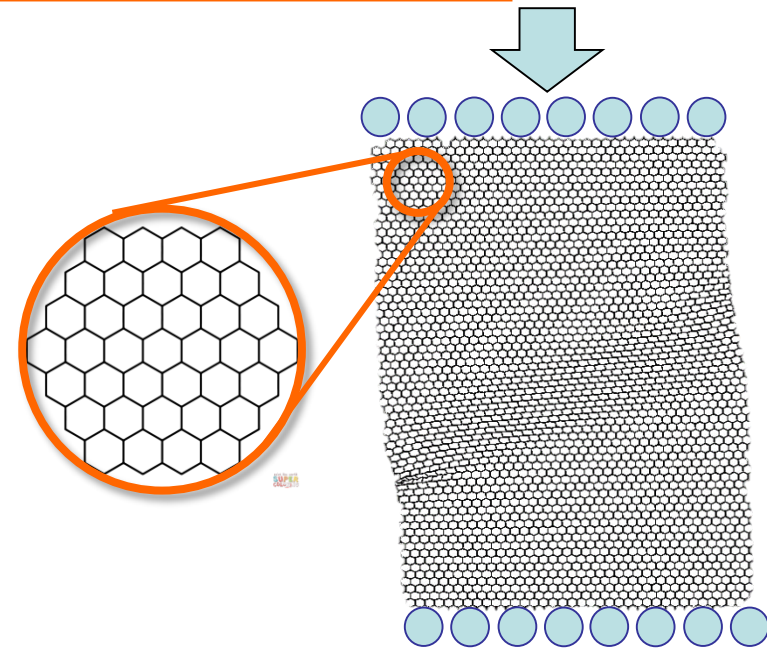


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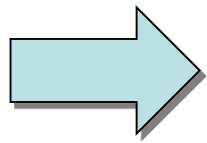
- Computational homogenisation (FE2)

- Heterogeneous structures
 - Micro-scale: cell, grains, inclusions...
 - Macro-scale: seen as a continuum
- Direct numerical simulations
 - Time consuming
- Idea: use multi-scale strategy



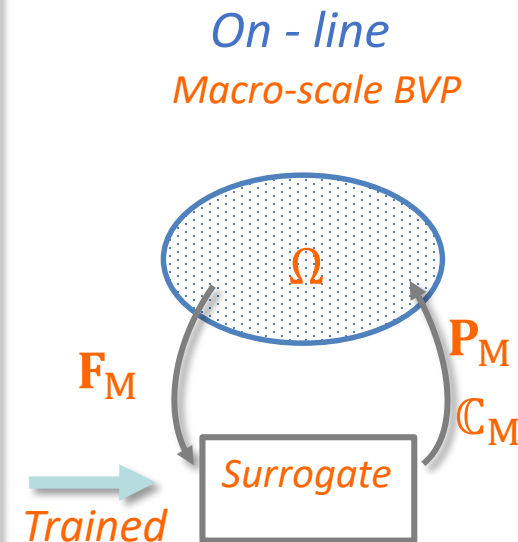
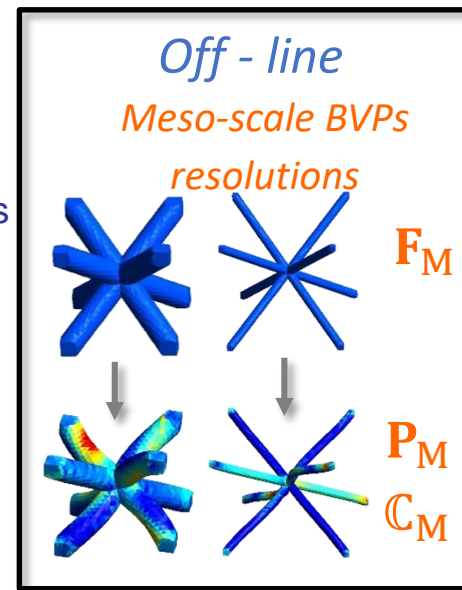
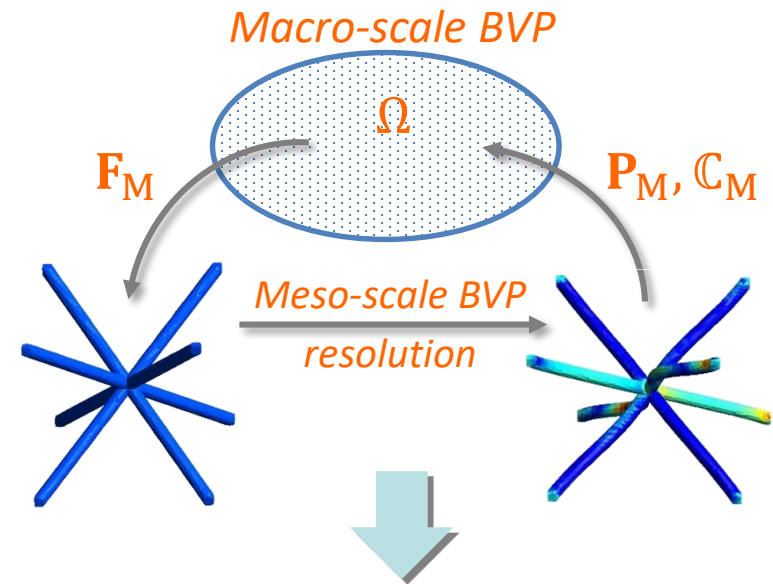
- Computational homogenisation (FE2)

- Non-linear simulations
 - Iterations at macro-scale BVP
 - Sub-iterations at meso-scale BVP



Unaffordable

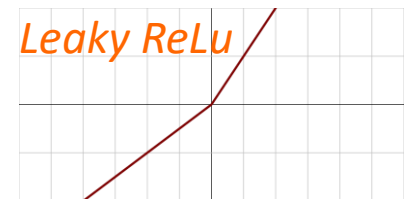
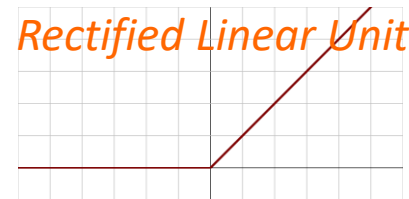
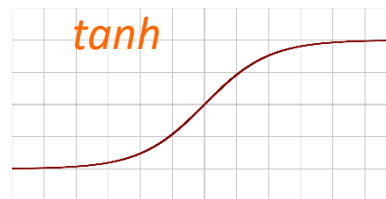
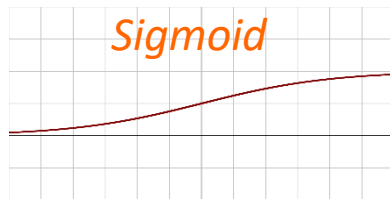
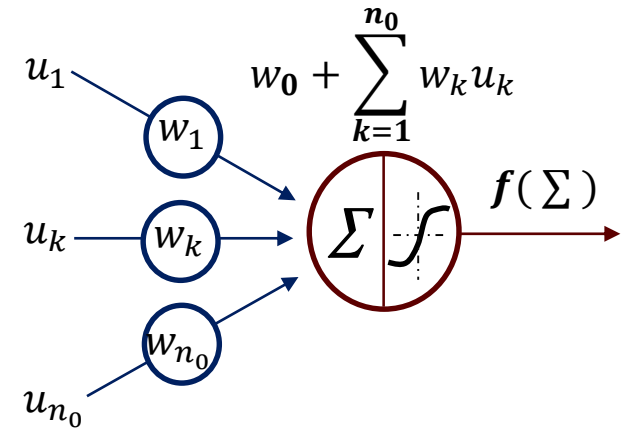
- Introduction of data-driven approach
- Use of surrogate models
 - Train a surrogate model (off-line)
 - Requires extensive data
 - Obtained from RVE simulations
 - Use the trained surrogate model during analyses (on-line)
 - Speed-up of several orders



Artificial Neural Network

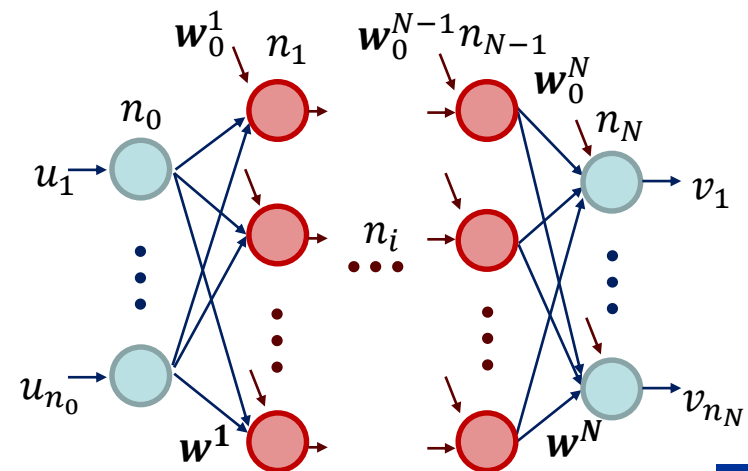
- Definition of the surrogate model

- Artificial neuron
 - Non-linear function on n_0 inputs u_k
 - Requires evaluation of weights w_k
 - Requires definition of activation function f
- Activation functions f



- Feed-Forward Neuron Network

- Simplest architecture
- Layers of neurons
 - Input layer
 - $N - 1$ hidden layers
 - Output layers
- Mapping $\mathbb{R}^{n_0} \rightarrow \mathbb{R}^{n_N}: v = g(u)$



• Training

– Evaluate

- The weights w_{kj}^i , $k = 1..n_{i-1}, j = 1..n_i$
- The bias w_0^i
- Minimise error prediction \mathbf{v} vs. real $\mathbf{v}^{(p)}$

$$L_{\text{MSE}}(\mathbf{W}) = \frac{1}{n} \sum_i^n \left\| \mathbf{v}_i(\mathbf{W}) - \mathbf{v}_i^{(p)} \right\|^2$$

- Requires an optimizer: Stochastic Gradient Descent

$$\Delta \mathbf{W} = -\mathcal{F} \left(\frac{\partial L_i(\mathbf{W})}{\partial \mathbf{W}}, \left(\frac{\partial L_i(\mathbf{W})}{\partial \mathbf{W}} \right)^2, \text{batch size, ...} \right)$$

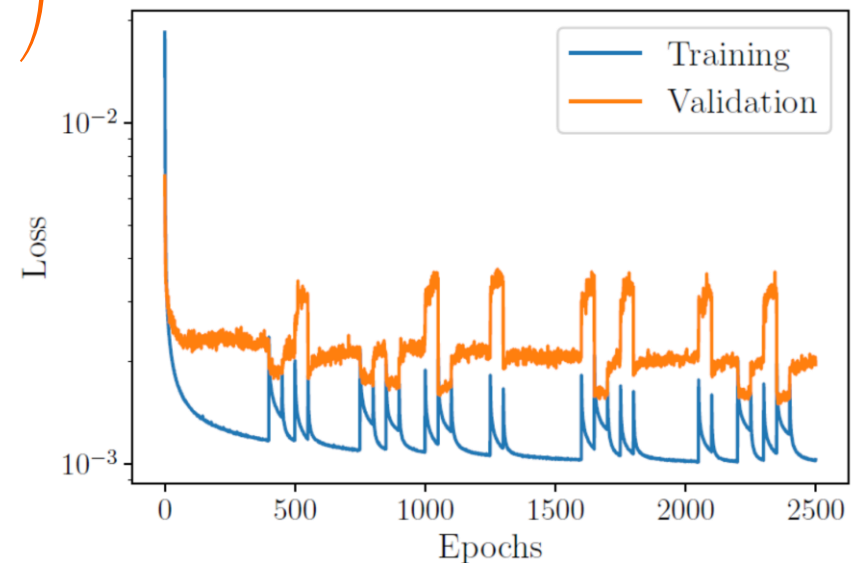
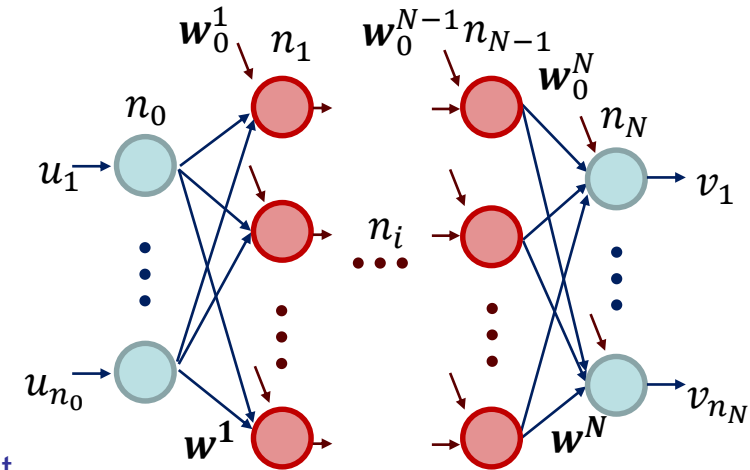
– Training data

- Input $\mathbf{u}^{(p)}$ & Output $\mathbf{v}^{(p)}$

• Testing

– Use new data

- Input $\mathbf{u}^{(p)}$ & Output $\mathbf{v}^{(p)}$
- Verify prediction \mathbf{v} vs. real $\mathbf{v}^{(p)}$

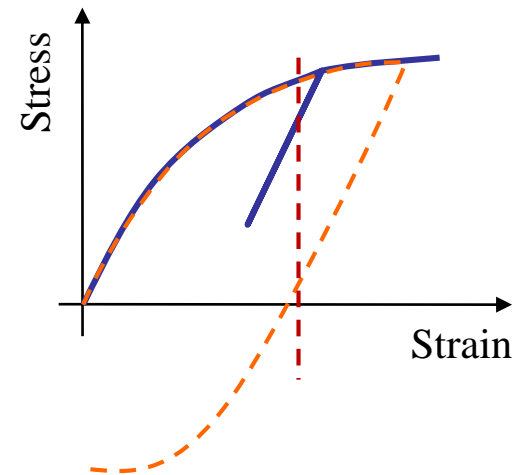
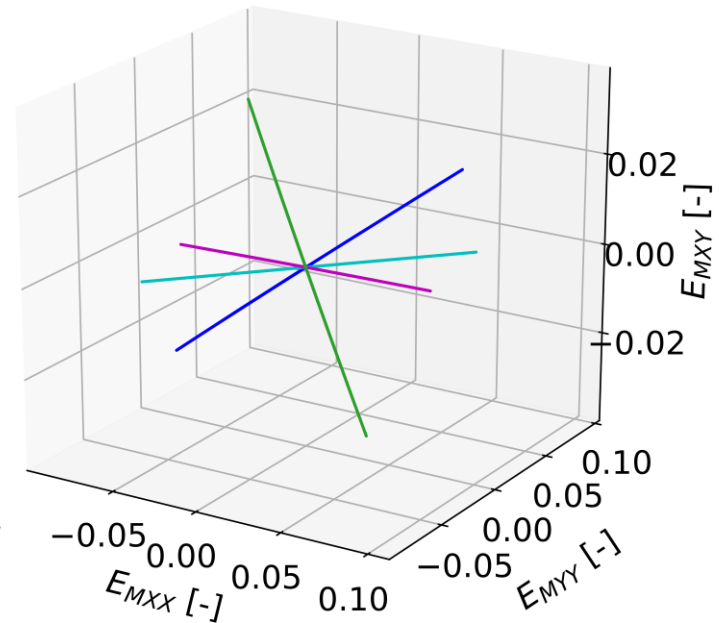


- Input / output definition

- Input:
 - Strain (history): \mathbf{F}_M
- Output:
 - Stress (history): \mathbf{P}_M

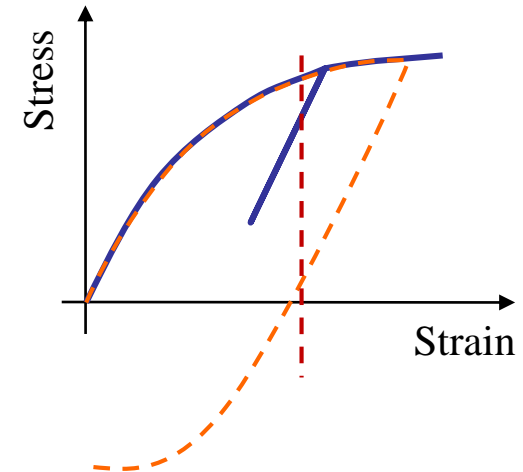
- Methodology

- Address problem of history dependency
 - RVE without buckling
 - Elasto-plastic composite RVE



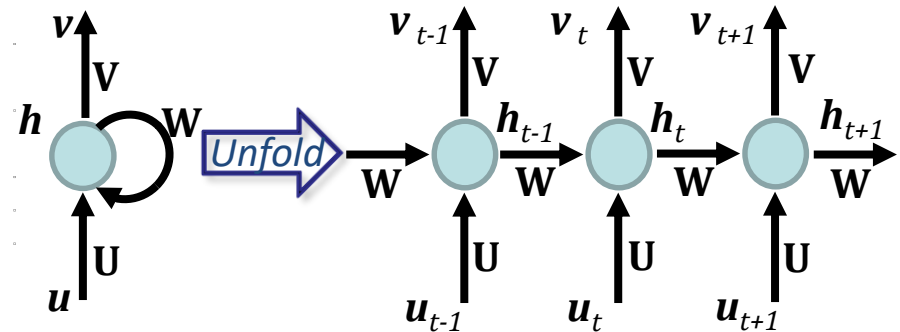
- Elasto-plastic material behaviour

- No bijective strain-stress relation
 - Feed-forward NNW cannot be used
 - History should be accounted for



- Recurrent neural network

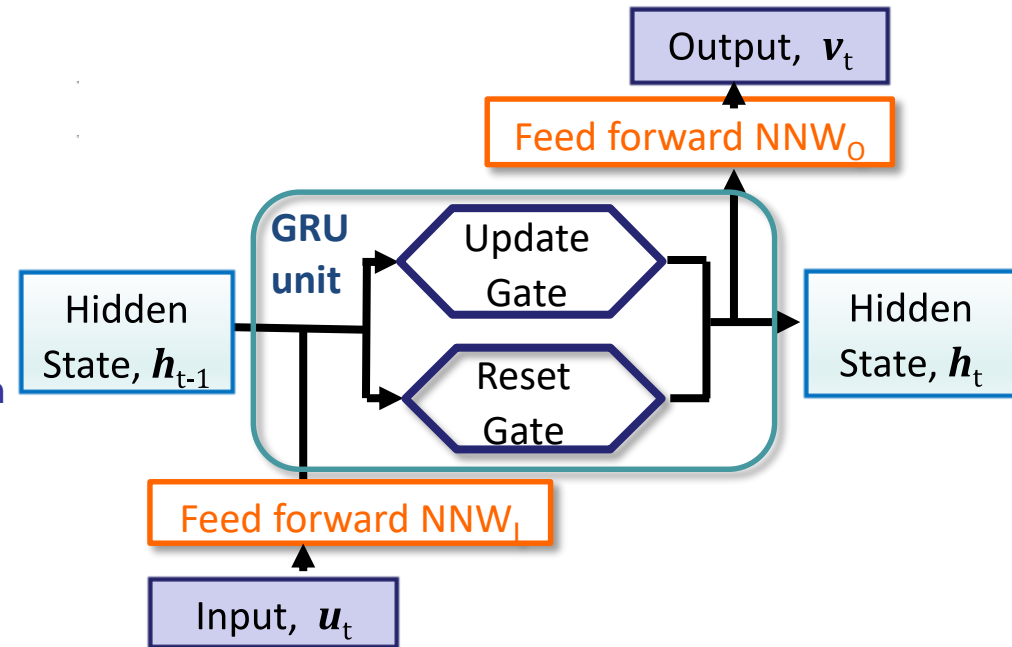
- Allows a history dependent relation
 - Input u_t
 - Output $v_t = g(u_t, h_{t-1})$
 - Internal variables $h_t = g(u_t, h_{t-1})$
- Weights matrices U, W, V
 - Trained using sequences
 - Inputs $u_{t-n}^{(p)}, \dots, u_t^{(p)}$
 - Output $v_{t-n}^{(p)}, \dots, v_t^{(p)}$



- Recurrent neural network design

- 1 Gated Recurrent Unit (GRU)

- Reset gate: select past information to be forgotten
- Update gate: select past information to be passed along
- Need to define number of hidden variables h_t

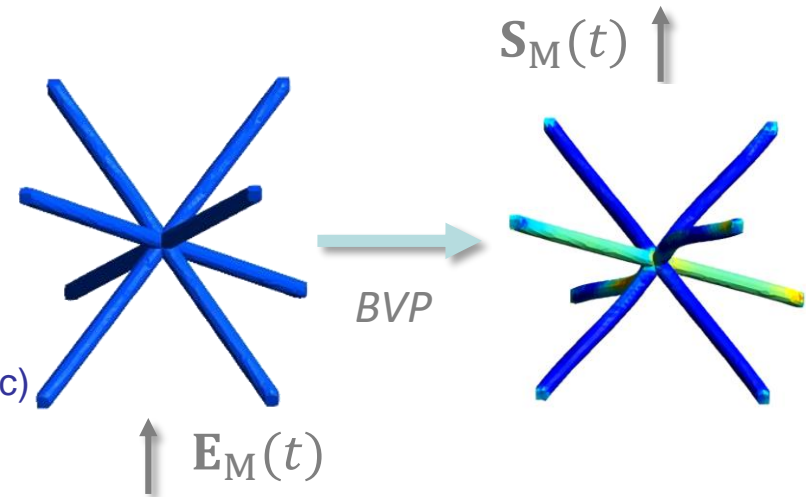


- 2 feed-forward NNWs

- NNW_I to treat inputs u_t
- NNW_O to produce outputs v_t

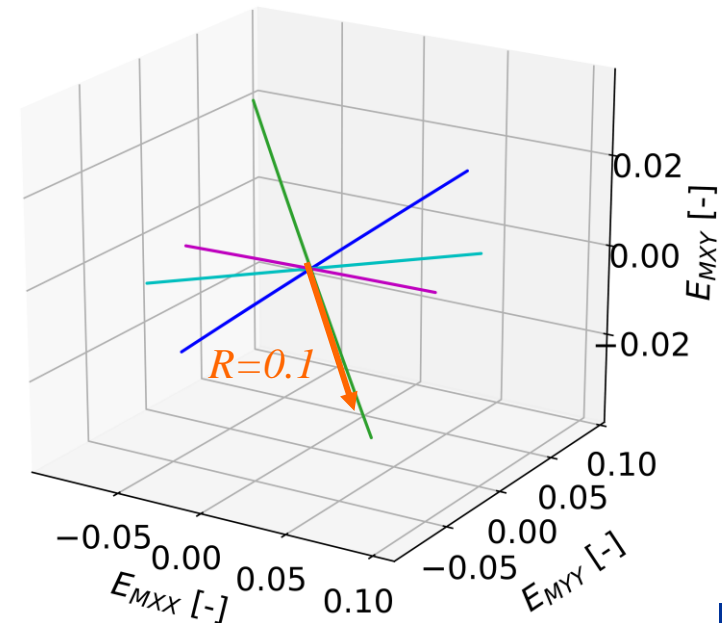
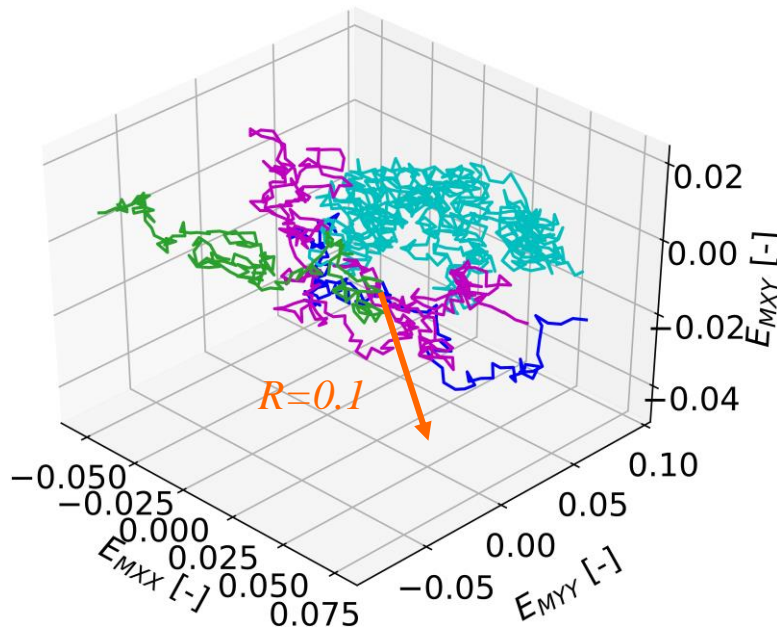
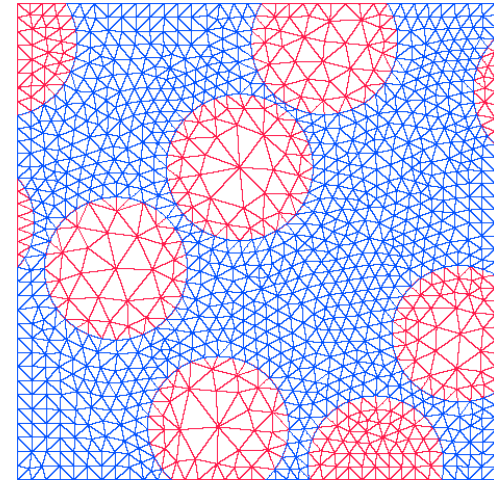
- Input and Output

- u_t : homogenised GL strain E_M (symmetric)
- v_t : homogenised 2nd PK stress S_M (symmetric)



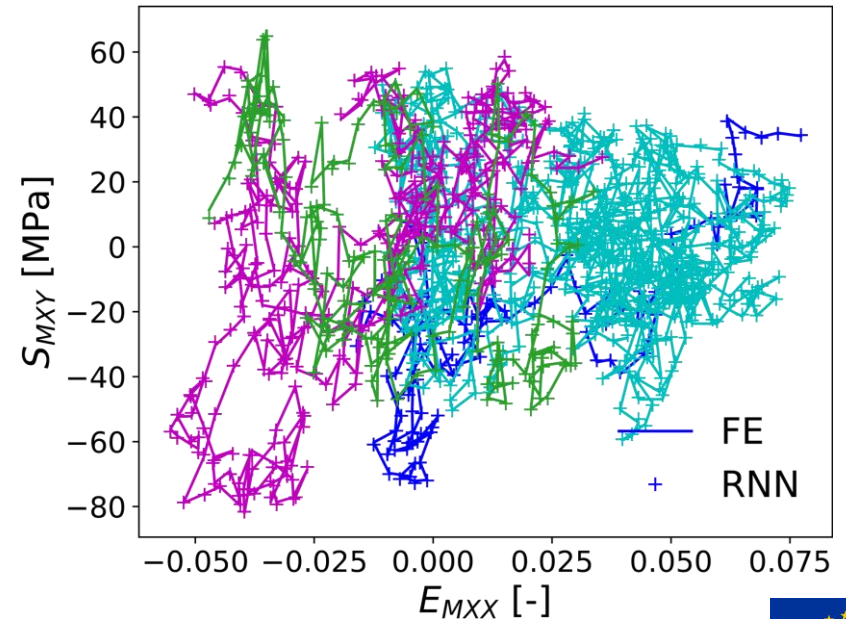
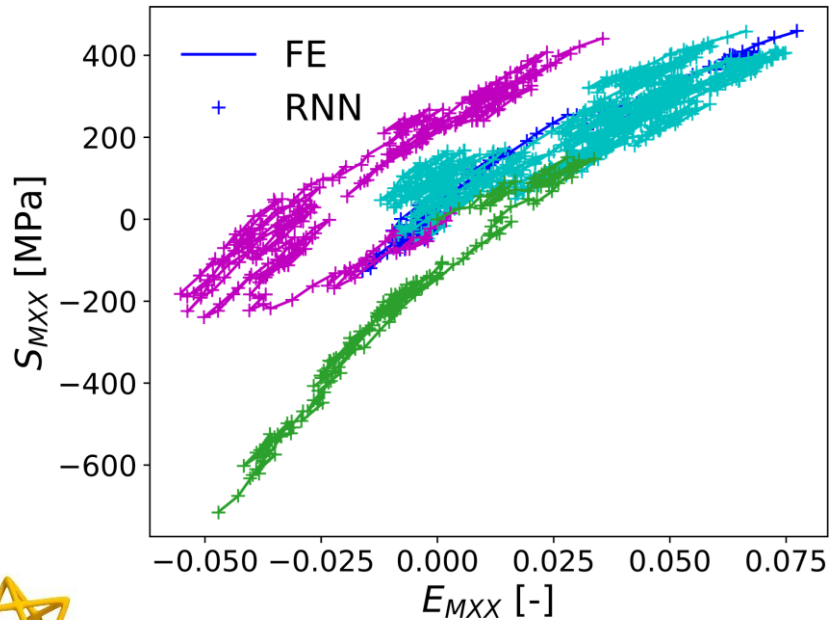
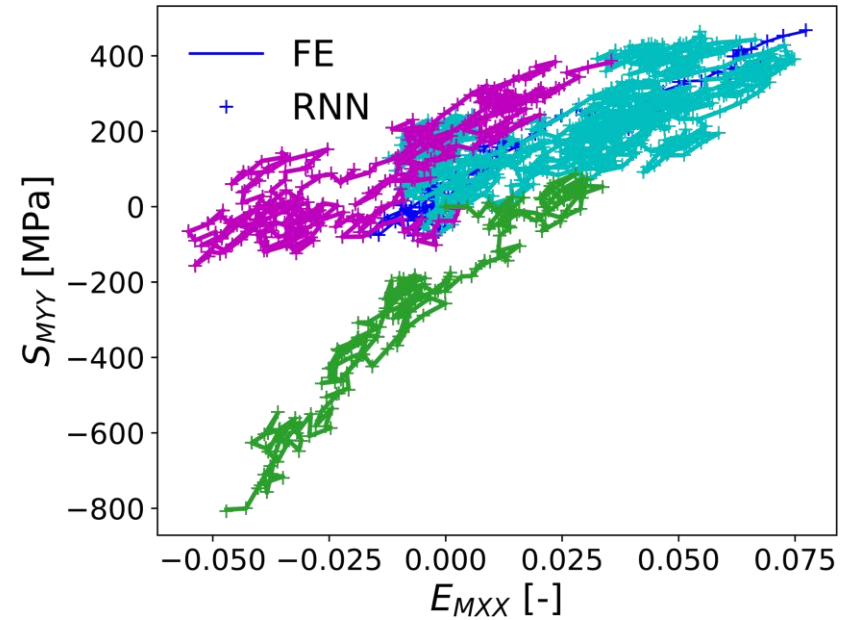
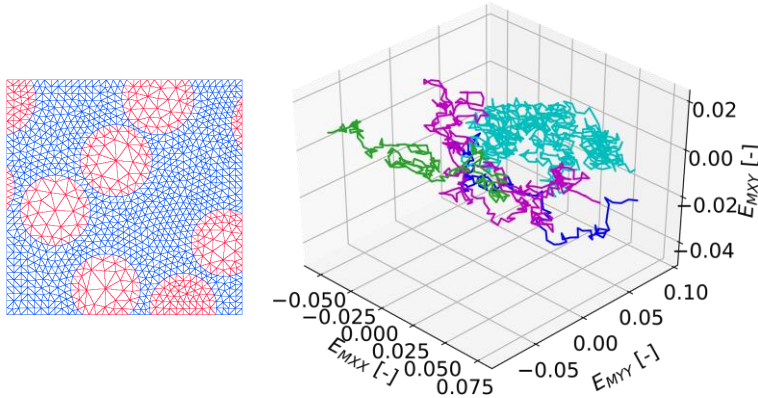
- Data generation

- Elasto-plastic composite RVE
- Training stage
 - Should cover full range of possible loading histories
 - Use random walking strategy (thousands)
 - Completed with random cyclic loading (tens)
 - Bounded by a sphere of 10% deformation



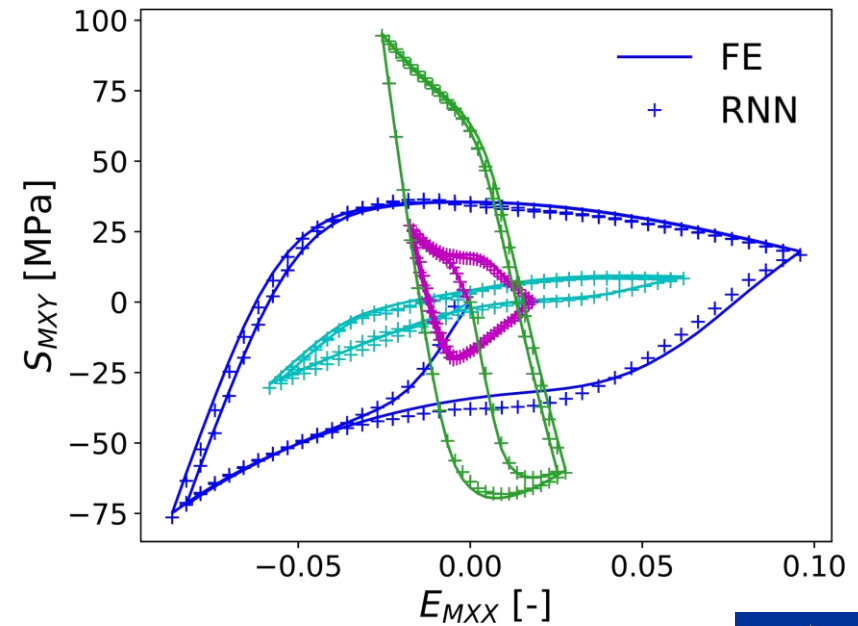
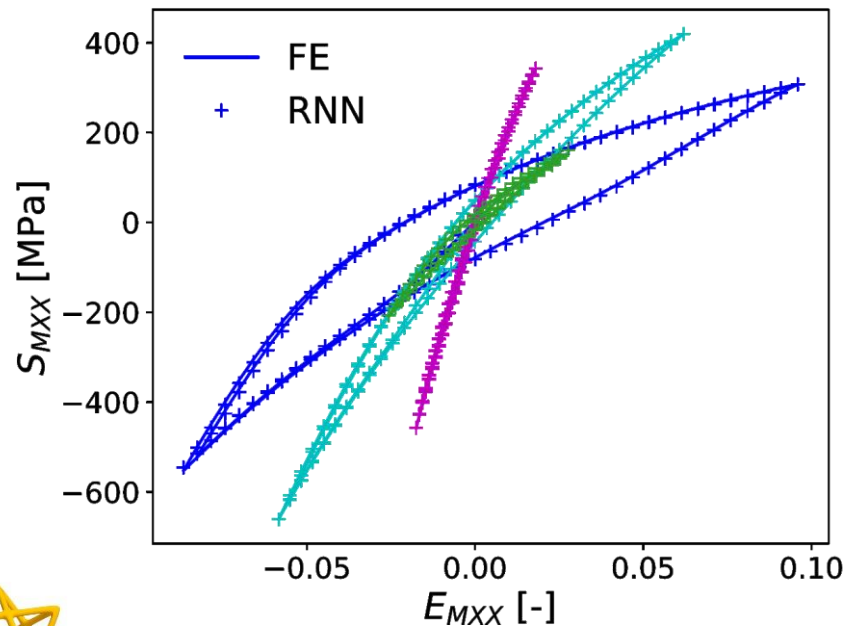
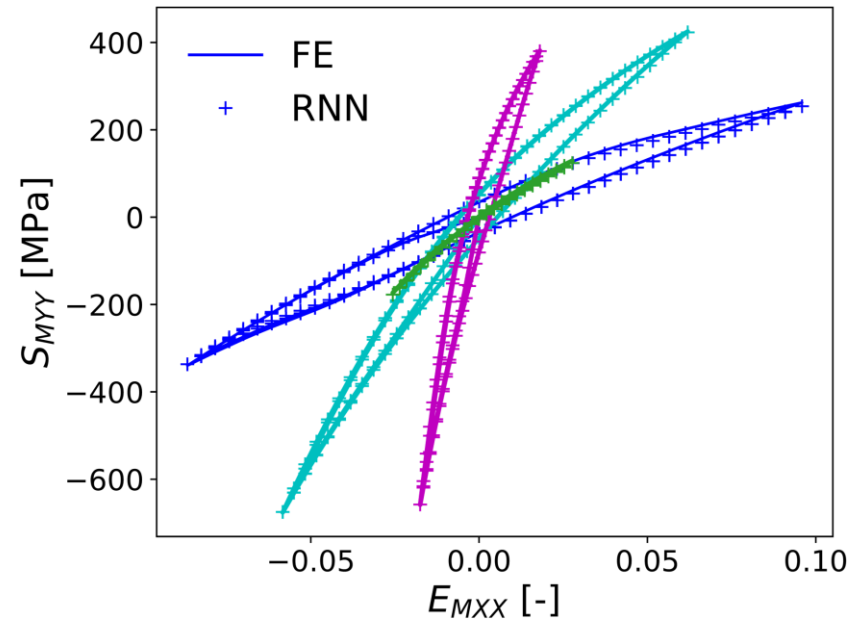
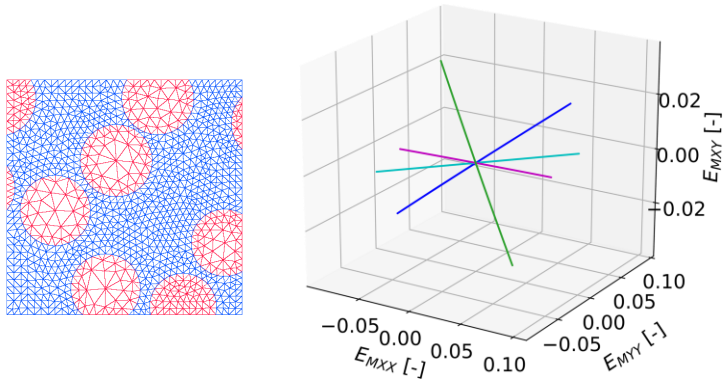
- Testing process (new data)

- On random walk



- Testing process (new data)

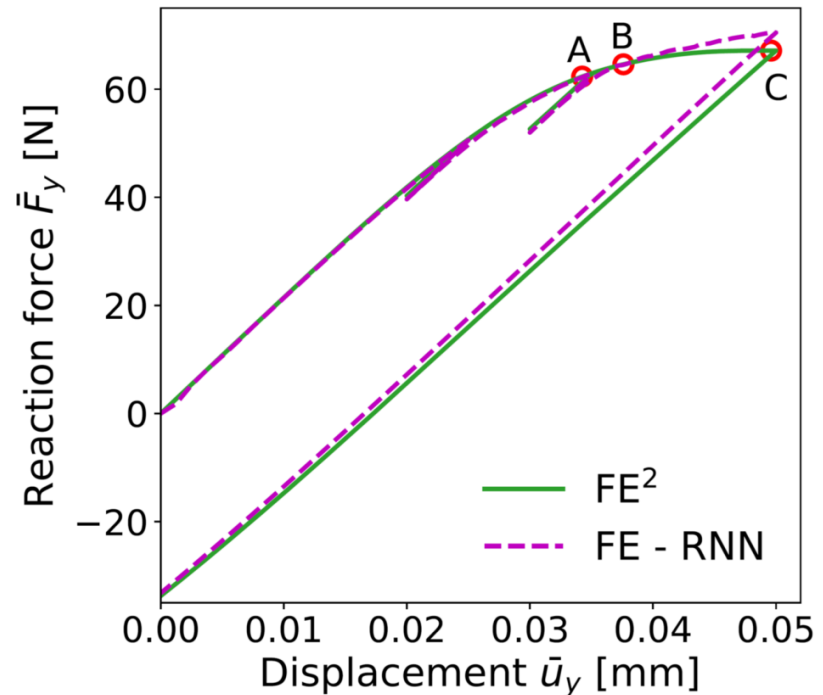
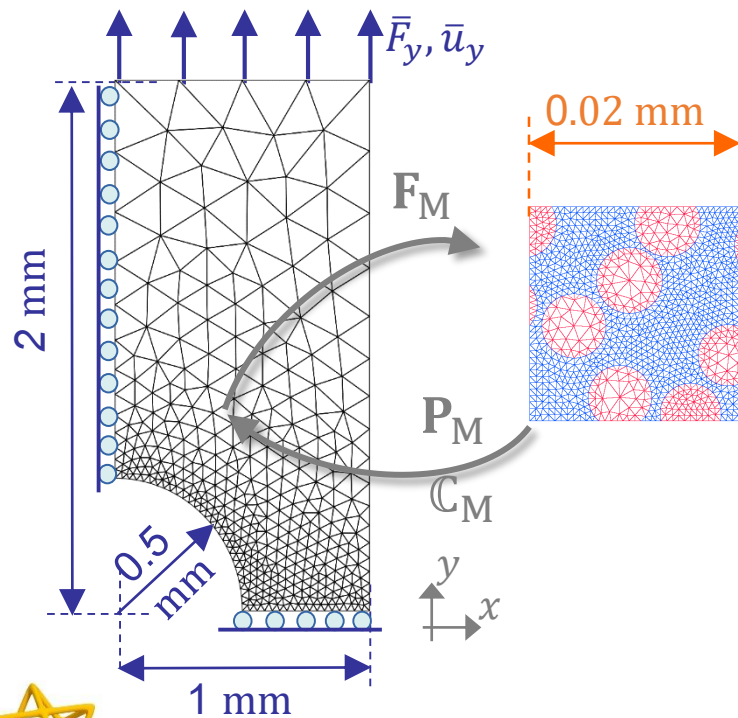
- On cyclic loading



Multiscale simulation

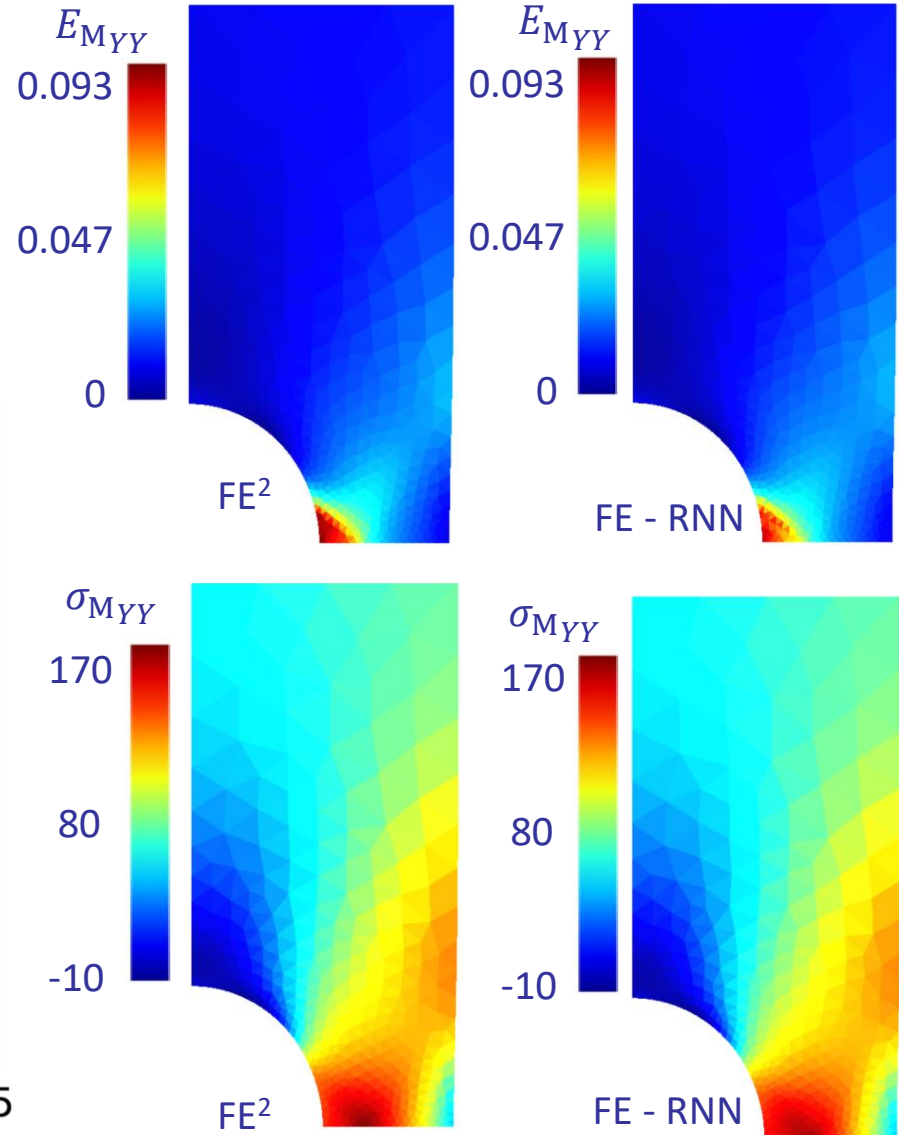
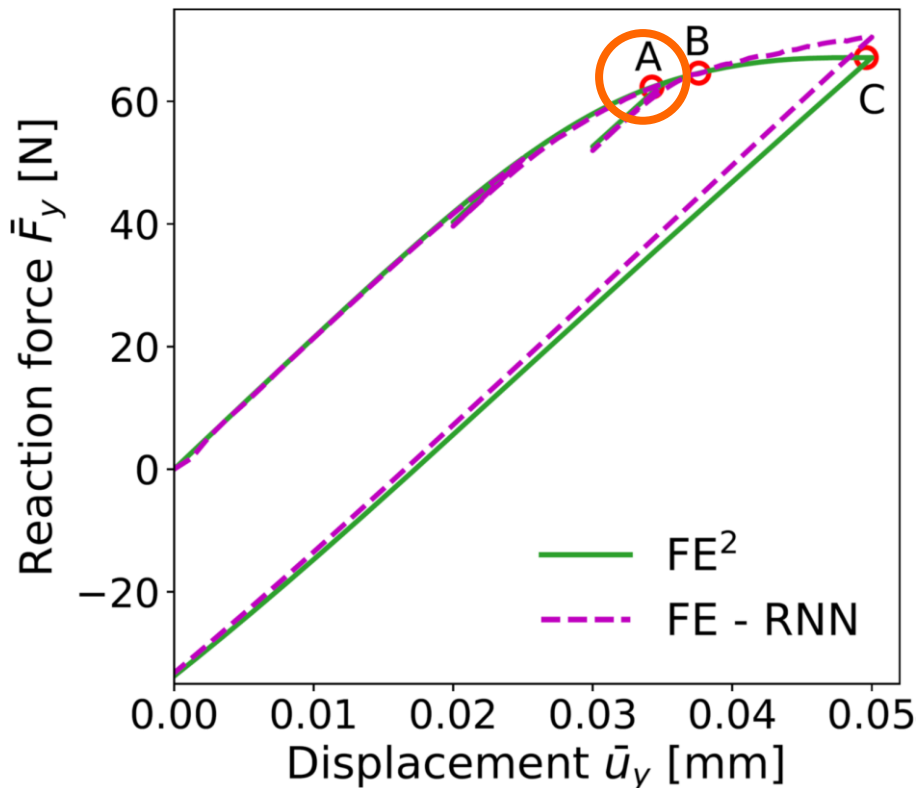
- Elasto-plastic composite RVE
- Comparison FE^2 vs. RNN-surrogate
- Training data
 - Bounded at 10% deformation

Off-line	FE^2	FE-RNN
Data generation	-	9000 x 2 h-cpu
Training	-	3 day-cpu
On-line	FE^2	FE-RNN
Simulation	18000 h-cpu	0.5 h-cpu



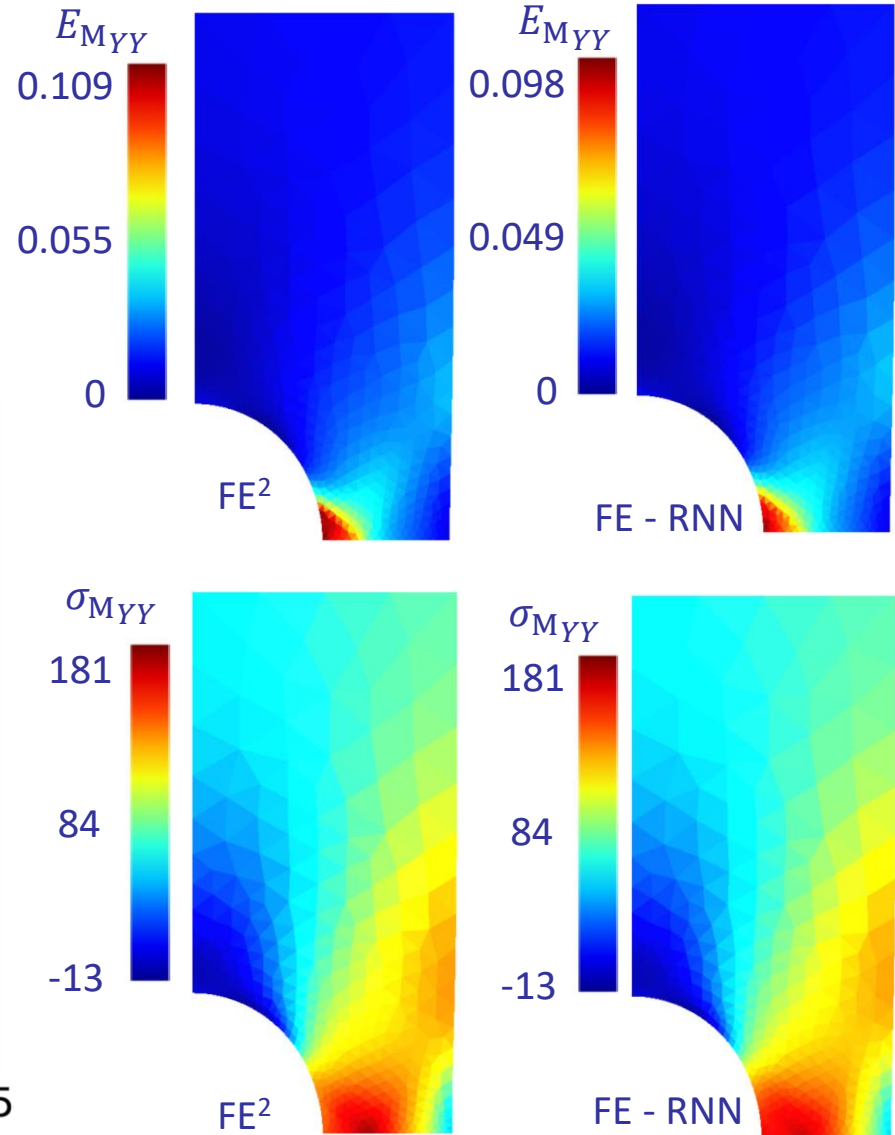
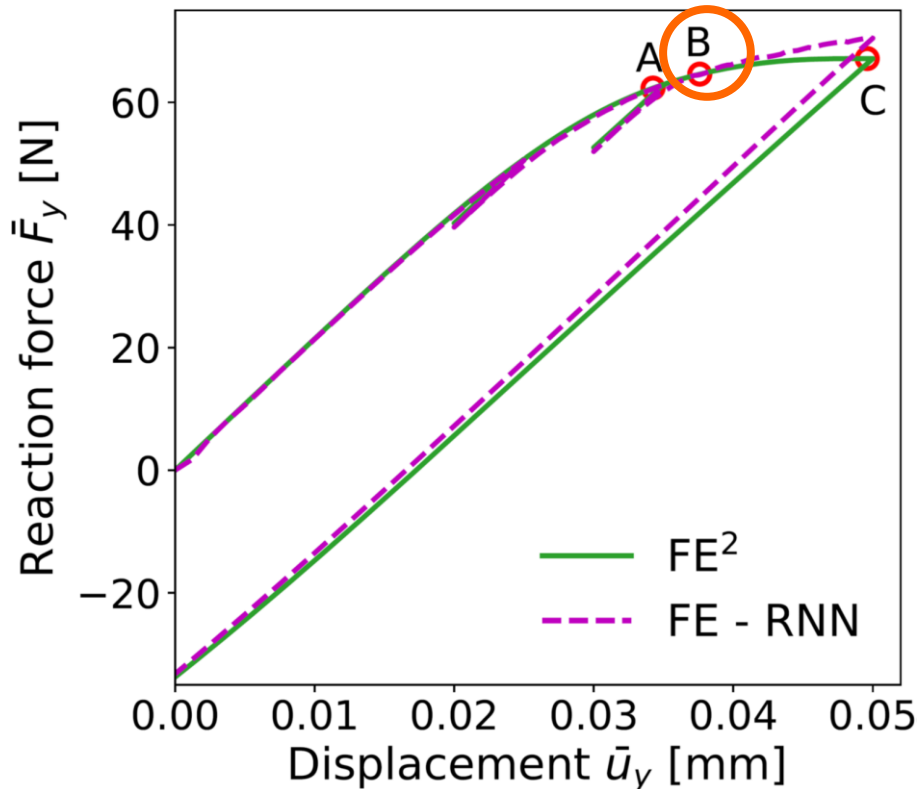
- Multiscale simulation

- Stress-strain distribution at point A
- Strain within the 10% training range



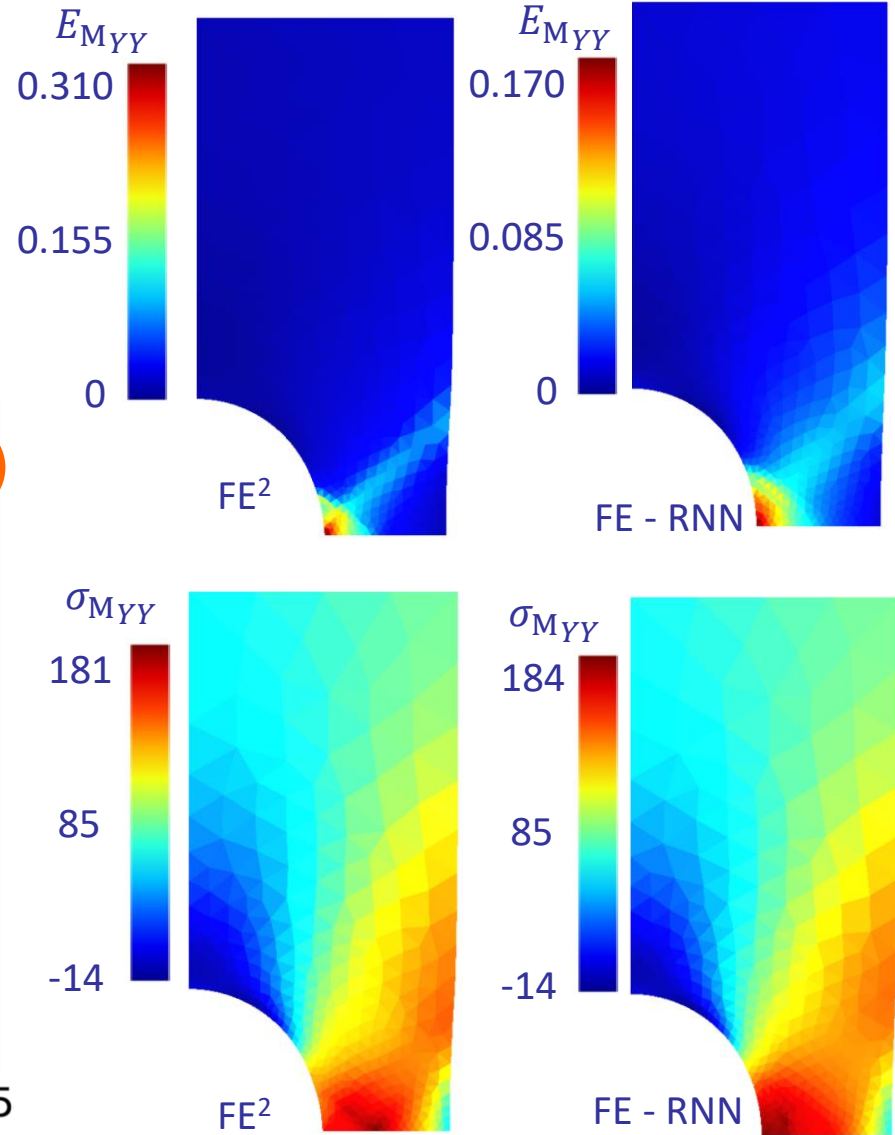
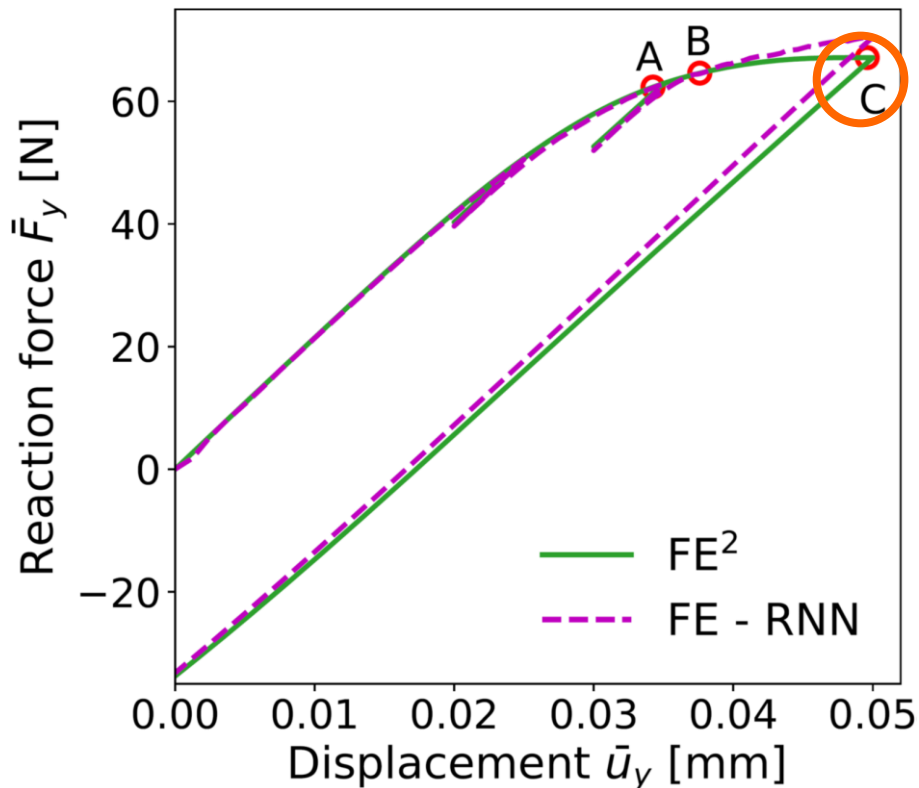
- Multiscale simulation

- Stress-strain distribution at point B
- Strain just at 10% training range



- Multiscale simulation

- Stress-strain distribution at point C
- Strain out of 10% training range

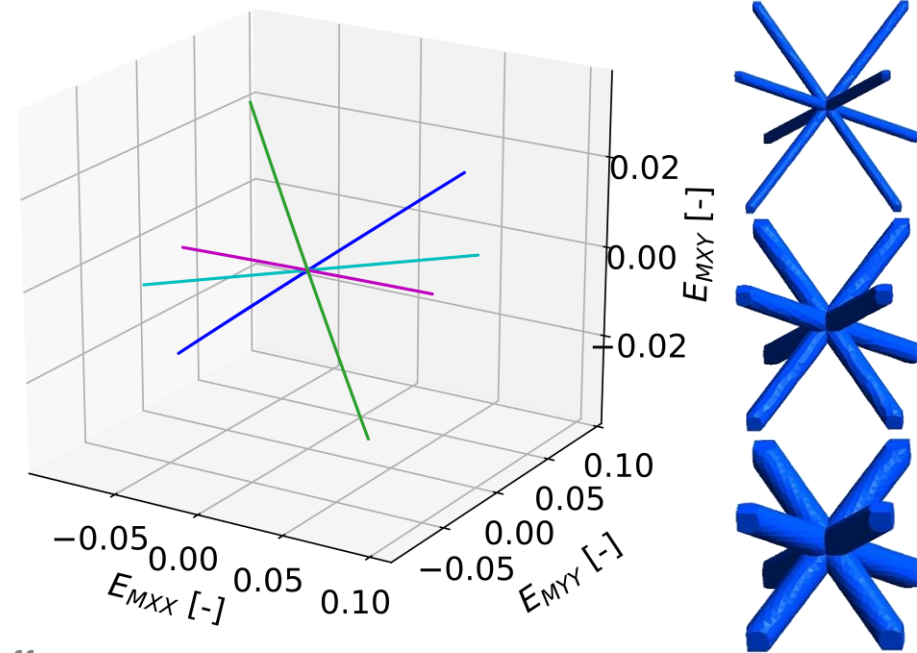


- Input / output definition

- Input:
 - Strain (history): \mathbf{F}_M
 - Geometry/material parameters: φ_m
- Output:
 - Stress (history): \mathbf{P}_M

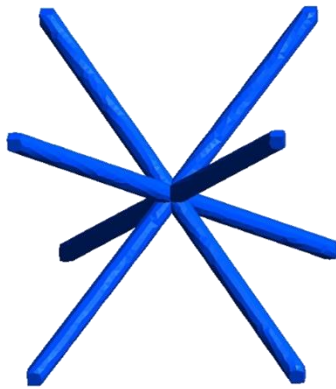
- Methodology

- Address problem of geometry/material effect
 - Octet cells
 - Elastic material at first

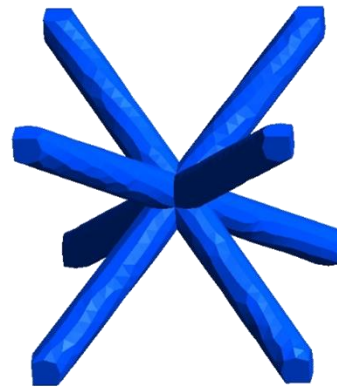


- Octet cell

- Generalised IMDEA script to generate random cells and random loading paths



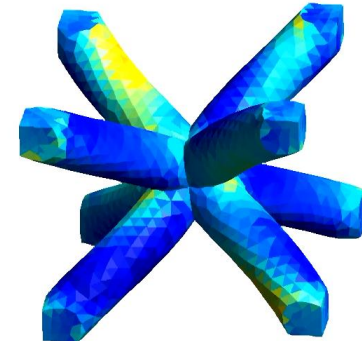
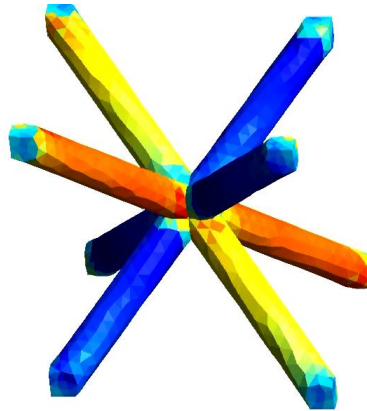
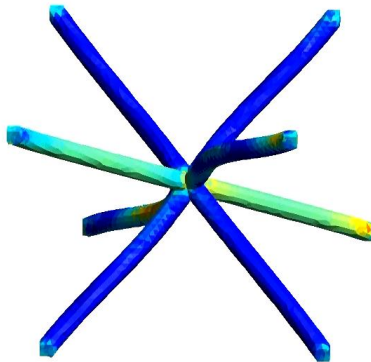
$V_f = 0.046; l = 1.70 \text{ mm}$



$V_f = 0.095; l = 1.72 \text{ mm}$

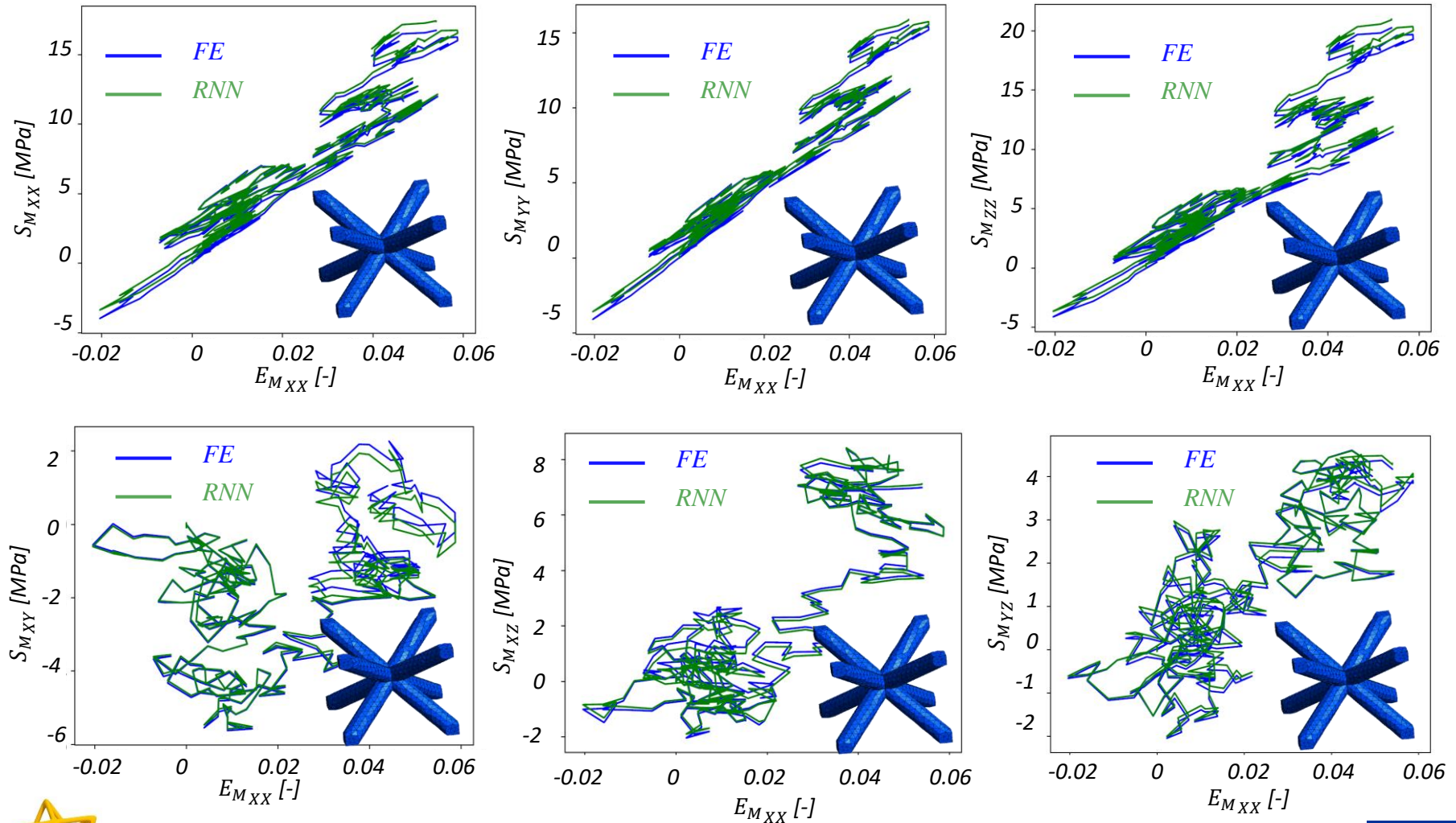


$V_f = 0.18; l = 1.50 \text{ mm}$



- Octet cell

– Test on new random cell/path

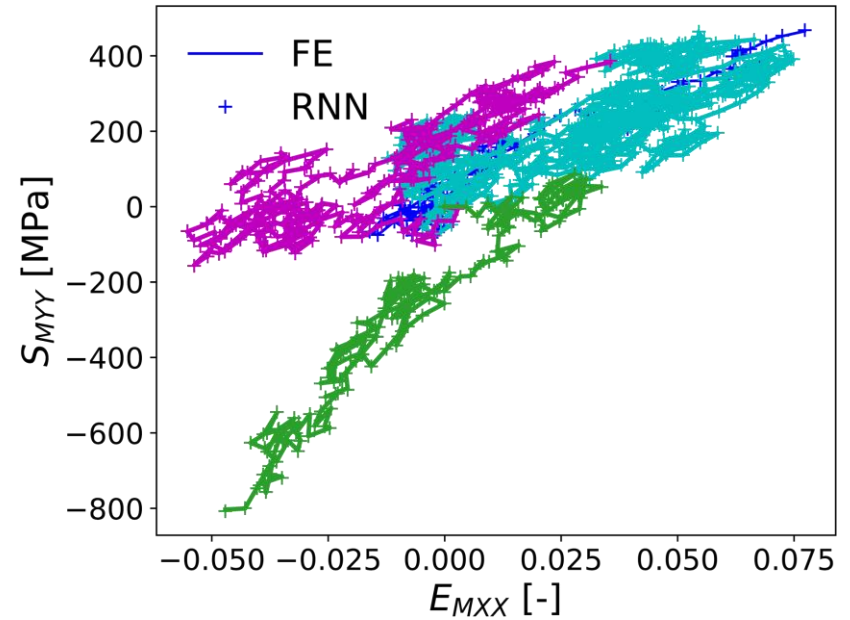
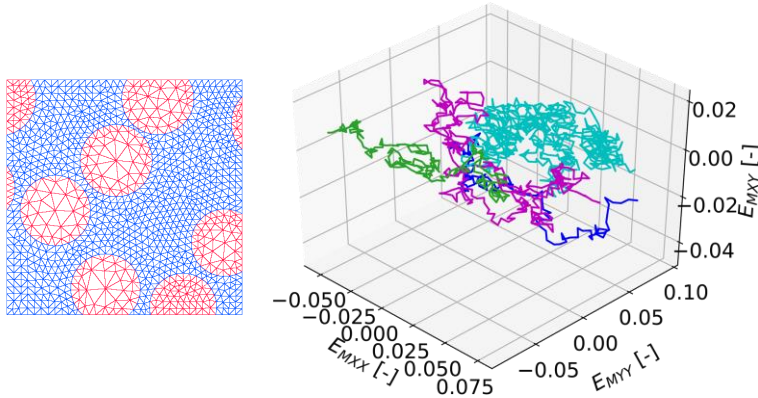


- More on
 - www.moammm.eu
 - L. Wu, V. D. Nguyen, N. G. Kilingar, and L. Noels. "A recurrent neural network-accelerated multi-scale model for elasto-plastic heterogeneous materials subjected to random cyclic and non-proportional loading paths." Computer Methods in Applied Mechanics and Engineering 369 (September 1, 2020): 113234, <http://dx.doi.org/10.1016/j.cma.2020.113234>



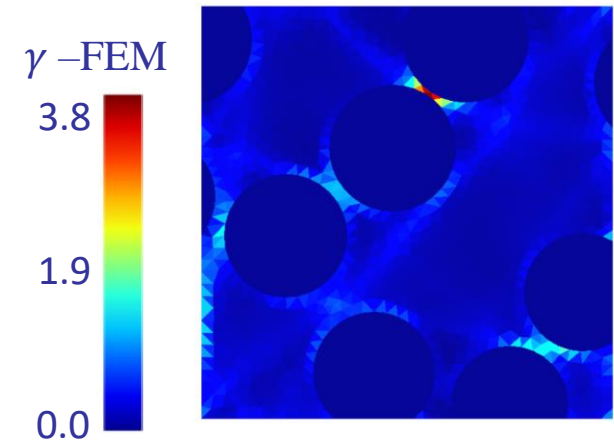
- Only homogenised output is predicted

- On random walk



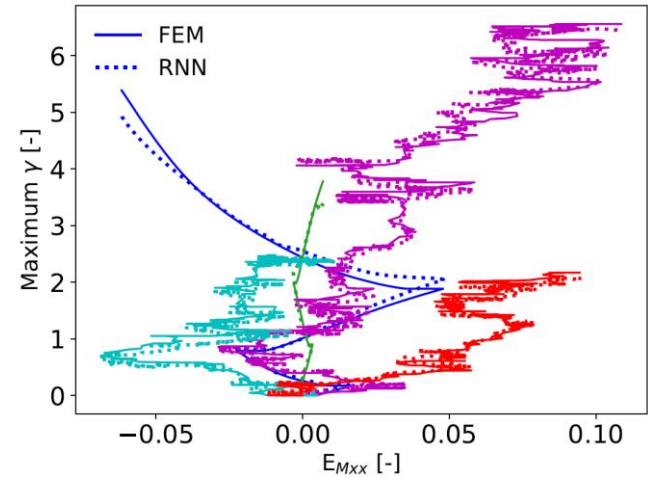
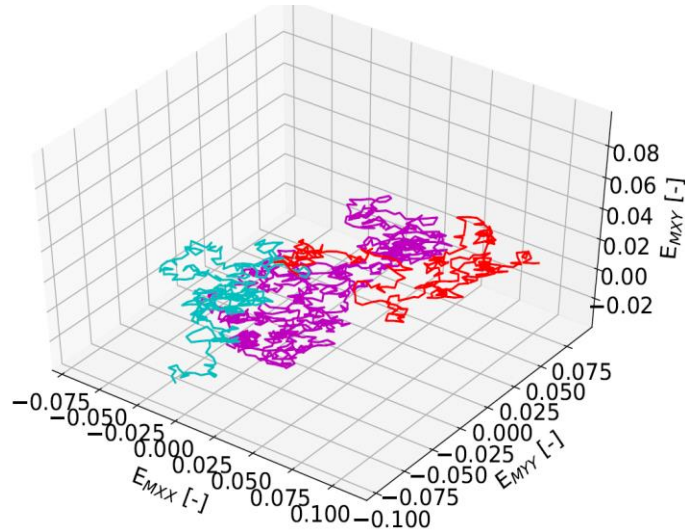
- Quid of local fields?

- This is an advantage of multiscale methods
- Useful to predict failure, fatigue etc.
- Can we get it back at low cost?



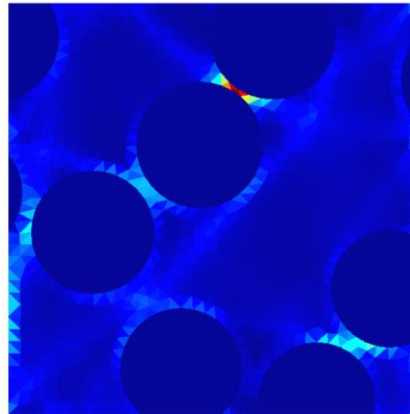
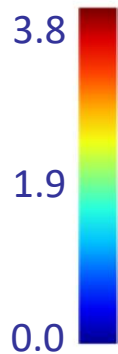
Localisation step

- Evaluation of equivalent plastic strain γ : Random loading (testing data)

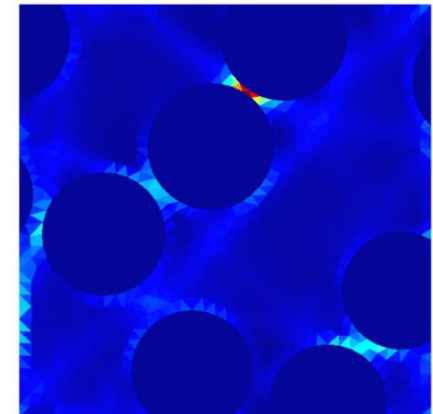


Purple loading –
step 500

γ –FEM



γ –RNN



Localisation step

- Evaluation of equivalent plastic strain γ : Cyclic loading (testing data)

